Crystal Growth by Physical Vapor Transport

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Physical vapor transport (PVT) offers several advantages (e.g., lower process temperature, improved purity and stoichiometry) over other techniques of bulk crystal growth. The quality of the crystals may, however, be downgraded by the presence of convection in the growth system. Another source of crystal imperfections may be interactions (sticking) of the crystal with the walls of the growth capsule. Our research program addresses these topics.

Growth of crystals by "contactless" PVT (without contact with the side walls of the growth ampoule) depends on such factors as the geometry of the ampoule and furnace, their configuration, temperature field, thermal and thermochemical properties of the materials (crystal, ampoule), composition of the vapor phase, type of medium outside the ampoule, and others. The technique of "contactless" PVT in compact geometry (the diameter of the crystal is close to that of the ampoule) has been used in the past. However, the literature reports on the subject are primarily experimental, and no comprehensive treatment of the method exists. The technique could be very useful for a prospective experiment(s) performed under microgravity conditions: elimination of crystal defects generated by crystal-wall interactions would improve the crystal quality and facilitate (or even enable) identification of gravity-related effects. The project consists of the following tasks:

- Theoretical and experimental determination of the mass transport properties of the Pb (Se, Te) (lead selenide-telluride) and (Cd, Zn) Te (cadmium-zinc telluride) model materials;
- Numerical fluid-dynamic modeling of the growth system; and
- Crystal growth experiments.

Since the initiation of the project (May 1995), thermochemical analysis of PVT of Pb (Se, Te) has been done; experimental verification of the model is under way. The technique for determining residual gases in sealed ampoules (important for a meaningful description of the actual growth conditions) has been developed. Purification procedures for the source materials (removal of oxygen) have been determined theoretically and verified experimentally. Two furnaces suitable for visual monitoring of the growth process have been fabricated. Numerical modeling of the thermal field in the system has been initiated.

To investigate the convective effects in PVT, a suitable growth system for terrestial and microgravity experiments is necessary. Such a system should enable a meaningful comparison of the theoretical predictions of convective effects with experimental results. That requires the geometry that would be feasible for a realistic modeling of the fluid flow and crystal growth in the ampoule. The main technical problem here is how to maintain a flat crystal-vapor (c-v) interface for the duration of the experiment. The shape of the interface is a complex function of the system parameters, particularly the geometry, temperature field, thermal and thermochemical properties of the materials, and the growth rate. With the aid of numerical modeling, different ampoule designs, materials, and other process conditions will be tested and their effect on the shape of the c-v interface will be anticipated. The theoretical predictions will be verified experimentally.

Another important task of the project is to develop a growth system which will provide a means for identifying convective flows during growth. This will be accomplished by using an appropriate doped binary and/or ternary source materials and investigating the distribution of the minority component(s) in the grown crystal.

Our research program is aimed at a better understanding of the role of convection and its significance for crystal growth from the vapor. The results of this work will provide the basis for designing a related microgravity experiment on convective phenomena in vapor growth systems. The results of the work may be also beneficial for industrial applications of the PVT technique.

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Biographical Sketch: Dr. Martin Volz is a research scientist in the Space Sciences Laboratory, and is currently working in the area of semiconductor crystal growth and characterization.